Journal of Molecular Structure (Theochem), 256 (1992) 315
Elsevier Science Publishers B.V., Amsterdam

AUTHOR INDEX

Alagona, G., 187
Ángyán, J.G., 113
Åqvist, J., 135
Arteca, G.., 125

Barakat, M.T., 75
Bhattacharjee, A.K., 61
Brinck, T., 29

Catálan, J., 161
Chau, P.-L., 75
Cocchi, M., 217

Dean, P.M., 75
Desideri, A., 153
Dot, T., 287
De Benedetti, P.G., 217, 231
de Paz, J.L.G., 161

Eckert-Maksić, M., 271

Fabero, F., 161
Falconi, M., 153
Ferenczy, G.G., 113, 249

Ghio, C., 187
Grice, M.E., 29
Guha, S., 61

Hodošček, M., 271
Horikoshi, K., 47

Jayasuriya, K., 17

Kikuchi, O., 47
Koritsánszky, T., 113

Lopez de Briñas, E., 287

Majumdar, D., 61
Maksić, Z.B., 271
Manaut, F., 287
Menziani, M.C., 217
Mezey, P.G., 125
Murray, J.S., 29

Nagy, J., 113
Náray-Szabó, G., 113
Nilsson, O., 295

Pèpe, G., 175
Politzer, P., 29
Polticelli, F., 153

Reboul, J.-P., 175
Reynolds, C.A., 249
Richards, W.G., 249
Rupnik, K., 271

Sanz, F., 287
Sawaryn, A., 91
Scheiner, S., 1
Siri, D., 175
Sokalski, W.A., 91

Takahashi, I., 47
Tapia, O., 295

Journal of Molecular Structure (Theochem), 256 (1992) 317–318
Elsevier Science Publishers B.V., Amsterdam

SUBJECT INDEX

Applied electric fields
Similarities between the effects of configurational changes and applied electric fields on the shape of electron densities, 125

Biomolecules
Modelling of ion–ligand interactions in solutions and biomolecules, 135

Carbonic anhydrase
Electronic and electrostatic aspects of carbonic anhydrase inhibition by sulphonamides, 217
Configurational changes
Similarities between the effects of configurational changes and applied electric fields on the shape of electron densities, 125
Cu, Zn superoxide dismutase
An electrostatic enzyme–substrate recognition: the case of Cu, Zn superoxide dismutase, 153
Cumulative multicenter multipole moment databases
Cumulative multicenter multipole moment databases and their applications, 91

Drug design
The molecular electrostatic potential and drug design, 175
Development of quantitative methods for studying electrostatic complementarity in molecular recognition and drug design, 75

Enzyme–substrate recognition
An electrostatic enzyme–substrate recognition: the case of Cu, Zn superoxide dismutse, 153
Ether-type oxygen
Rapid evaluation of molecular electrostatic potential maps by simple analytical functions.
Application to compounds containing ether-type oxygen atoms, 47
Experimentally-based reactivity indices
Correlations between molecular electrostatic potentials and some experimentally-based indices of reactivity, 29

5-HT ligands
Complete or partial comparison of molecular potential distributions? Some tests with 5-HT ligands, 287
Hydrogen bonds
On the underlying source of energetics of bending of hydrogen bonds, 1

Ion–ligand interactions
Modelling of ion–ligand interactions in solutions and biomolecules, 135

Molecular recognition
Development of quantitative methods for studying electrostatic complementarity in molecular recognition and drug design, 75

NH_2 group
A theoretical study of the resonance effect by means of the NH_2 group, 161

Personal computers
Protein electrostatics on personal computers, 113
Pharmacological properties
Molecular electrostatic potential: a tool for the prediction of the pharmacophoric pattern of drug molecules, 61
Phosphaalkynes
A computational investigation of phosphaalkynes: a new building block, 17
Polyglycine 87-mers
Electrostatic forces and the structural stability of a modelled bacteriophage T4 glutaredoxin fold: molecular dynamics simulations of polyglycine 87-mers, 295
Potential derived charges
Methods for determining the reliability of semiempirical electrostatic potentials and potential derived charges, 249
Proteins
Protein electrostatics on personal computers, 113

Resonance effect
A theoretical study of the resonance effect by means of the NH_2 group, 161

Semiempirical electrostatic potentials
Methods for determining the reliability of semiempirical electrostatic potentials and potential derived charges, 249

Solute–solvent interactions
The role of electrostatics in solute–solvent interactions with the continuum, 187

Structure–activity relationship
Electrostatics in quantitative structure–activity relationship analysis, 231

Sulphonamides
Electronic and electrostatic aspects of carbonic anhydrase inhibition by sulphonamides, 217

T4 glutaredoxin
Electrostatic forces and the structural stability of a modelled bacteriophage T4 glutaredoxin fold: molecular dynamics simulations of polyglycine 87-mers, 295

Vitamin C
Intra- and extra-molecular electrostatic potentials in vitamin C, 271